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1 On the impact of porous media microstructure on
2 rainfall infiltration of thin homogeneous green roof
3 growth substrates

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10 **Abstract**

Green roofs are considered an attractive alternative to standard storm water management methods; however one of the primary issues hindering their proliferation is the lack of data regarding their ability to retain and reduce storm water under a variety of climatic conditions. This lack of data is partly due to the complexity of physical processes involved, namely the heterogeneous microscopic behavior that characterize flows in unsaturated porous media. Such an anomalous behavior is difficult to predict a priori, especially in the presence of layered structures. This paper examines water infiltration of a green roof at the pore-scale with the aim to evaluate the effect of the porous microstructure in thin substrate layers. In such layers, the thickness of the medium and the particle size are within the same order of magnitude and the effect of the packing arrangement on the flow dynamics can be pronounced. In this study, three packing arrangements and two different hydraulic heads, analogous to extreme rainfall events typical of Scandinavia, are investigated by means of direct numerical simulations based on the lattice Boltzmann

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method. The results show that a wider variability of pore sizes in a thin medium can be linked directly to flow pathing preference and consequently less homogenized flow in the primary flow direction. This situation corresponds to intermittent flow behavior at the pore-scale level and reduced macroscopic infiltration rates. This observation unveils the possibility of designing innovative green roof growth substrates: by tuning the particle size and thickness of the layers composing the medium the desired green roof detention time can be attained.

11 *Keywords:* Green roof; Lattice Boltzmann; microstructure; rainfall;
12 infiltration; substrate

13 **1. Introduction**

14 Climatic predictions in northern latitudes indicate a long-term overall in-
15 crease in rainfall intensity and frequency, leading to increased flooding risks
16 in urban environments [1]. This trend and its effects such as urban flooding
17 have already been recorded in Scandinavia as well as felt across Europe and
18 beyond. Due to the cost and difficulty associated with modification of exist-
19 ing storm water management networks it is necessary to examine alternative
20 methods by which excess storm water can be detained and removed. One
21 such candidate is the use of green and blue roofing in urban environments,
22 capable of efficient infiltration, detention and drainage of storm water. Green
23 roofs are defined as any roofing structure that incorporates living vegetation
24 in a growth substrate and commonly additional layers for drainage, a root
25 barrier and waterproofing. Blue roofs are specifically intended for storm wa-
26 ter management and may incorporate several of the layers mentioned above,

27 however they may not be vegetated. The use of green roofs reduces additional
28 spatial planning in urban environments for storm water drainage and catch-
29 ment that would otherwise be necessary. By using the rooftops it is possible
30 to achieve greater vegetated areas in cities without significant disruption to
31 the systems and structures already in place.

32 There already exists significant interest in the use of green and blue roofs
33 internationally for a variety of reasons. These reasons range from urban
34 pollution and noise reduction [2] to urban heat island reduction [3]. With the
35 inclusion of their use for urban storm water management it is understandable
36 that interest for the installation of such roofs is increasing, though there
37 remain a few hindrances to the development and implementation of such
38 installations. The primary factor impeding the growth in interest and use
39 of green and blue roofs lies in the lack of sufficient available quantified data.
40 The data of primary interest consists of peak runoff delay time and quantity
41 reduction, total retention capacity, time required for evaporative drying of
42 the soil, and thermal properties. This type of information is difficult to
43 obtain as it is highly dependent upon prior water saturation levels in the
44 soil, soil material composition and compaction, plant type, and temperature
45 to name the largest factors. If we consider only storm water detention, this
46 performance data is relevant not only to city planners and the producers
47 themselves but also to the building designers who must take into account
48 the structural implications of fully saturated roofs. The secondary issue is
49 the higher price of such constructions and regular maintenance schedules
50 required to keep the roofs in good health.

51 These issues can be addressed by the determination of storm water in-

52 filtration, detention and drainage through these constructions. Storm water
53 detention encompasses the delay and peak flow reduction of runoff through-
54 out and after a rainfall event by the mechanical process of liquid infiltration
55 of the soil. Alternatively, retention covers the reduction of runoff by the pro-
56 cesses of capturing infiltrating water in the pore structure and its subsequent
57 removal by way of evaporation and transpiration, including the contribution
58 of vegetation. Previous research on this topic is primarily experimental and
59 covers laboratory scale experiments through full-scale green roofs. A heavily
60 important factor in the performance of green roofs is evapotranspiration as
61 outlined in [4, 5] due to the nature of liquid storage in porous soil substrates.
62 While this physical phenomenon cannot be ignored when discussing the long-
63 term performance of green roofs, the time scale over which it operates makes
64 it of little use in short-term extreme rainfall events, which are of primary
65 importance. Studies by Hamouz et al. [6] and Stovin et al. [7] have found
66 that while green roofs perform well on isolated rainfall events with regard
67 to retention and detention of storm water they are less effective over several
68 events in close temporal proximity, particularly if one or more events are of
69 a greater intensity. Of particular note is that retention of storm water is
70 severely reduced by prior rainfall events and the best one can generally hope
71 for is simply a detention within the system.

72 Other experimental work on green roofs has focused on the plant ecology
73 [8, 9] with the aim of greater climatic resilience and possible additional ben-
74 efits to storm water performance in terms of evapotranspirative efficiency. A
75 final aspect of experimental research is the determination of the growth sub-
76 strate material composition on detention and retention performance. Work

77 by Stovin et al. [9] has shown that different mixes of substrate materials has
78 a measurable impact on the performance, suggesting substrate composition
79 can be modified to improve performance. A further point of note of these
80 studies is the state of the growth medium with regard to prior wetting and
81 current liquid presence on the imbibition and drainage of subsequent storm
82 water.

83 Beyond the use of more commonplace hydrological models such as HY-
84 DRUS, SWMM and similar efforts [10, 11] there has been little work on the
85 application of more detailed numerical modeling to accurately predict storm
86 water flow in green roofs. The modeling techniques of best notoriety are tra-
87 ditional computational fluid dynamics (CFD) using finite volume and finite
88 element methods. These modeling methods are ideal for use in the predic-
89 tion of infiltration and drainage dynamics as well as in aiding the roof design
90 and optimization for a variety of climatic conditions. The largest drawback
91 of such models lies in accurately capturing the hysteresis observed in liquid
92 infiltration of porous media such as soil. The hysteresis is caused by the
93 interdependency of the liquid and gas phase flows on each other as well as
94 the pore network morphology of the solid matrix; and accurately modeling
95 this relationship remains an unresolved problem in the discipline [12].

96 The difficulty of characterizing the interaction between a liquid and a gas
97 within a pore network has led to the widespread use of the lattice Boltz-
98 mann method (LBM) for this problem. The method is advantageous for use
99 on problems such as this due to a variety of reasons. The method solves the
100 Boltzmann equation of particle motion at the mesoscopic scale and therefore
101 allows for efficient computation as well as ease of boundary condition defini-

102 tion in complex geometries. Another advantage is the ability of the method
 103 to provide excellent result resolution for such problems that are not easily
 104 handled by traditional CFD methods. Many researchers have focused their
 105 efforts on determining the interactions and relevant parameters responsible
 106 for the hysteresis and details can be found in [13, 14, 15]. These works at-
 107 tempted to construct unique functions relating a combination capillary pres-
 108 sure, saturation and liquid-gas interfacial area. Others have applied integral
 109 geometry to define pore structure influence on capillary flow in terms of an
 110 Euler characteristic [16]. What is clear is that there is a contribution from
 111 the pore morphology on the infiltration and drainage process that must be
 112 explored in more detail at the microstructural (pore) scale.

113 This work explores the effect of the microstructure of thin substrate layers
 114 on water infiltration dynamics at the pore scale by using LBM on 3 domains
 115 with dissimilar properties. The microstructure for each domain is modified
 116 through alteration of the particle diameter in a homogeneous packed bed
 117 analogous to a representative thin soil volume. We define a medium “thin”
 118 when the thickness of the medium and the particle size are within the same
 119 order of magnitude. The infiltration is driven by hydraulic pressure applied
 120 via standing surface water whose height is determined by rainfall data taken
 121 from Gothenburg, Sweden. The results indicate the microstructure can pos-
 122 itively and negatively impact the infiltration of water into a thin porous
 123 medium. This behavior can be explained by the concept of capillary barriers
 124 [17] determined by the energy balance in the pore network [18]. When the
 125 particle sizes are increased in relation to the thickness of the porous medium
 126 we see a decrease in flow homogeneity. When the porous medium is insuf-

127 ficiently thick the particle packing encourages inhomogeneous flow profiles,
128 and consequently gives rise phenomenon such as the capillary barrier in some
129 pore networks that alters the global rate of water infiltration. This observa-
130 tion suggests the possibility of controlling the green roof detention time in
131 green roofs by adopting an optimized layered structure in their design.

132 In section 2 the methodology for the geometry construction and numerical
133 simulations is detailed. Section 3 includes the results and accompanying
134 discussion and a conclusion is given in section 4.

135 2. Materials and methods

136 2.1. Lattice Boltzmann method

137 The Lattice Boltzmann method solves the Boltzmann transport equation
138 which consists of a phase space discretized into a lattice mesh and is selected
139 for this work for several reasons. These reasons stem from the fact that
140 the method operates on the micro and mesoscale and therefore inherits the
141 advantages from molecular dynamics and kinematic theory. These advantages
142 include efficient parallelization in computation and ease of handling
143 complex geometries due to the simplified nature of the boundary condition
144 requirements. More importantly, the method provides the ability to answer
145 fundamental questions regarding a given flow at great resolution. Each individual
146 lattice structure consists of a centroid and nodes on the convex shell
147 of the lattice geometry. Fictive particles travel between the nodes governed
148 by a probability assigned for travelling to each position on the lattice. The
149 probabilities are chosen based upon the lattice geometry and facilitate the
150 recovery of the macroscopic properties of the fluid. This allows for complex
151 boundaries to be defined with simplicity using bounce-back condition on the
152 boundaries, negating the need for mesh refinement at the boundaries as required
153 in traditional CFD modeling. The second reason for the application
154 of this method lies in its innate ease for parallelization with regard to computation.
155 Since the lattice mesh is defined in a grid pattern by definition the
156 computations can be distributed without loss of information, thus drastically
157 increasing the computational speed [19].

158 In this work a 3-dimensional regular cubic lattice with 18 nodes on the

convex shell and a centroid, written as D3Q19, is used. The lattice Boltzmann code has been previously used for several different applications. For a validation of the two-phase lattice Boltzmann algorithm, the reader is referred to [20]. The solved equation is given as

$$f_r(\mathbf{x} + \mathbf{c}_r \delta t, t + \delta t) - f_r(\mathbf{x}, t) = -\tau^{-1}(f_r(\mathbf{x}, t) - f_r^{eq}(\mathbf{x}, t)) + F_r \quad (1)$$

where $f_r(\mathbf{x}, t)$ is the distribution function at position \mathbf{x} and time t along the r -th direction; \mathbf{c}_r is the so-called discrete velocity vector along the r -th direction over time interval δt ; τ is the mean collision time and is related to kinematic viscosity by $\nu = c_s^2(\tau - 0.5\delta t)$. The fluid is forced by a body force F_r which mimics the effect of gravity. Such a force is defined following the approach defined by Guo et al. [21],

$$F_r = \left(1 - \frac{1}{2\tau}\right) w_r \left(\frac{\mathbf{c}_r - \mathbf{u}}{c_s^2} + \frac{\mathbf{c}_r \cdot \mathbf{u}}{c_s^4} \mathbf{c}_r \right) (\rho \mathbf{g}) \quad (2)$$

with \mathbf{g} representing gravitational acceleration and \mathbf{u} the fluid velocity. The equilibrium distribution function $f_r^{eq}(\mathbf{x}, t)$ takes the form

$$f_r^{eq} = w_r \rho \left(1 - \frac{\mathbf{u}_{eq} \cdot \mathbf{u}_{eq}}{2c_s^2} \right), \quad r = 1 \quad (3)$$

$$f_r^{eq} = w_r \rho \left(1 + \frac{\mathbf{c}_r \cdot \mathbf{u}_{eq}}{c_s^2} + \frac{(\mathbf{c}_r \cdot \mathbf{u}_{eq})^2}{2c_s^4} - \frac{\mathbf{u}_{eq} \cdot \mathbf{u}_{eq}}{2c_s^2} \right), \quad r = 2 - 19 \quad (4)$$

where w_r is the appropriate weighting parameter for the D3Q19 lattice; ρ is the density; c_s is the speed of sound; and \mathbf{u}_{eq} is the velocity used for defining the equilibrium distribution functions, which can differ from the fluid

hydrodynamic velocity, on the basis of the specific forcing scheme used. In the present work, we apply the Guo forcing formulation for implementing the gravitational force whereas we make use of the Shan-Chen force for simulating surface tension [22]. The macroscopic flow quantities density and velocity, (ρ, \mathbf{u}) are thus related to the hydrodynamic moments as the following:

$$\rho = \sum_r f_r \quad (5)$$

$$\rho \mathbf{u} = \sum_r \mathbf{c}_r f_r + 1/2 \rho \mathbf{g} + 1/2 F_{sc} , \quad (6)$$

and the equilibrium velocity is formulated as: [23]

$$\mathbf{u}_{eq} = \rho \mathbf{u} + (\tau - 1/2) F_{sc} \quad (7)$$

where F_{sc} is the Shan-Chen gas-liquid interaction force. A detailed discussion of the forcing schemes proposed by Shan-Chen and Guo can be found in Huang et al. [24]. The Shan-Chen model was developed to overcome the limitations of LBM in dealing with components of differing molecular mass as well as thermodynamic phase transitions [22]. It is an ideal choice since we are interested in the interaction of two immiscible fluids as well as the interaction of the microstructure with the fluids. Its fundamental feature is the addition of an inter-particle potential which adds attractive or repulsive properties in combination with the elastic collision force already present in previous models. The inter-particle force gives rise in the system to a non-ideal equation of state:

$$p = \rho c_s^2 + \frac{G}{2} c_s^2 \Psi^2, \quad (8)$$

191 where liquid and gas phases coexist at the thermodynamic equilibrium state.

192 The Shan-Chen force is given by:

$$F_{sc} = -G\Psi(\mathbf{x}, t) \sum_r w_r \Psi(\mathbf{x} + \mathbf{c}_r \delta t, t) \mathbf{c}_r \quad (9)$$

193 where G , valued -5.5 in this work, is the interaction strength between the

194 phases and $\Psi(\rho)$ is a density-dependent pseudo potential function. Negative

195 values of G define an attractive force and positive values a repulsive force.

196 The pseudo-potential function calculates effective mass locally:

$$\Psi(\rho) = 1 - e^{-\rho}. \quad (10)$$

197 The effective mass approaches ρ itself when its value is low and obtains a

198 saturation value when it is increased. It is capable of capturing the two

199 important characteristics of a non-ideal flow, namely the equation of state in

200 Eq.(8) and surface tension.

201 The fluid-solid interaction is determined by a moving gas-liquid contact

202 line. This contact line is characterised by a contact angle that is chosen

203 under equilibrium conditions, without external forces, as determined by the

204 Young's equation. The equilibrium contact angle is implemented through

205 spatial averaging of the density-dependent potential function. The force at

206 the solid wall (Ψ_{wall}) is calculated using the method proposed by De Maio et

207 al. [25] and is of the form:

$$\Psi_{wall} = N^{-1} \sum_N \Psi + \Delta_w \quad (11)$$

208 where Ψ is the density-dependent function and N the nearest fluid compu-
 209 tational nodes. This formulation enforces a fixed density gradient at the
 210 wall and by tuning the parameter representing surplus density, Δ_w , different
 211 contact angles can be represented at the desired lattice resolution. More in-
 212 formation regarding the relationship between Δ_w and the contact angle can
 213 be found in Benzi et al. [26].

214 We perform a validation of two-phase Poiseuille flow between parallel
 215 plates using the methodology described in detail by Yang and Boek [27].
 216 The results are compared to the analytical solution in Reza and Martin [28]
 in Figure 1 and the agreement is found to be very high.

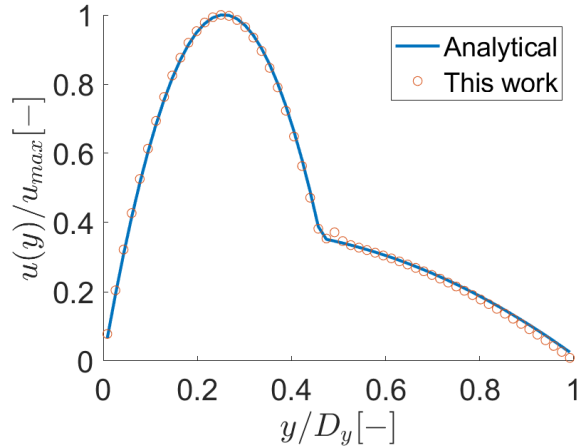


Figure 1: Comparison of the numerical framework used in this work against analytical solution by Reza and Martin [28], D_y is channel width. On the y axis the two-phase velocity normalized with the maximum velocity is shown.

217

218 2.2. Simulation setup

219 2.2.1. Domain specifications

220 The simulation domains are split into 2 sections; i) the surface liquid and
 221 ii) the porous medium consisting of a packed bed of homogeneous spher-

ical particles. The surface liquid section is a void and allows for the initialization of the wetting liquid without disruption to the porous medium below. A packed bed with uniform particle size (monodisperse) is chosen as an analogue to soil for this study so as to remove influence of particle inhomogeneities. These inhomogeneities include shape, orientation, surface roughness and hydrophilicity. These factors are neglected for this study in order to remove as much uncertainty as possible when analyzing the effect of particle packing on infiltration however in reality they contribute to the infiltration dynamics to a variable degree.

Three distinct packed beds of randomly packed homogeneous spherical particles of varying particle diameter are used for this study. A reference particle diameter was selected based upon a desired porosity and pore size reflecting the properties of lightweight expanded clay aggregate (LECA) [29]. This reference particle diameter d was converted from the given pore radius r_{eff} by applying the Revil, Glover, Pezard and Zamora (RGPZ) model [30, 31] which states

$$d = 2\Theta r_{eff}, \quad (12)$$

$$\Theta = \sqrt{\frac{ew^2}{8\epsilon_{ex}^{2w}}}, \quad (13)$$

where e is a model parameter valued $8/3$, w is the cementation exponent valued 1.5 for spherical particles and ϵ_{ex} is the experimentally determined porosity. The reference particle diameter is slightly varied to generate the other two particle diameters as listed in Table 1.

The height of the packed bed H is determined by the representative vol-

243 ume requirement for the porous medium with particle sizes as previously
 244 defined. The particle diameter is chosen as a characteristic length as it deter-
 245 mines the pore microstructure within the porous region. A new parameter ϕ
 246 representing the packing effect of the particles on the microstructure is given
 247 by

$$\phi = \frac{H}{d}. \quad (14)$$

248 This quantity will be used to define the three different cases of packing ar-
 249 rangements and is one of the two primary parameters in this study. The
 250 values of ϕ are listed in Table 1.

251 The packed bed length perpendicular to the flow direction, L , is chosen
 252 such that it adheres to restrictions regarding wall effects on the calculated
 253 flow field [32]. The boundaries perpendicular to the primary flow direction
 254 must be at least 15-20 times the particle diameter to ensure wall effects are
 255 negated.

256 The packed beds were generated using the software Blender, which is
 257 capable of applying basic rigid body physics to objects and tracking their
 258 motion in time. Particles of a specified diameter are dropped into a box,
 259 which is later removed in the computation stage of this work. This method
 260 for creation of packed bed domains has been outlined and validated by Boc-
 261 cardo et al. [33] and is an efficient tool for this purpose. A binary lattice
 262 is generated for each domain by calculating each node's distance from the
 263 particle centers and defining the node accordingly. The information for the
 264 3 domains is given in Table 1 and an example is plotted in Figure 2. Here ϵ
 265 is the porosity calculated over the domain for each case.

Table 1: Packed bed domain physical properties.

ϕ	6.7	10.1	5.1
$L \times L \times H$ [mm]	$15 \times 15 \times 5$	$15 \times 15 \times 5$	$15 \times 15 \times 5$
d [mm]	0.740	0.494	0.986
ϵ	0.389	0.377	0.40

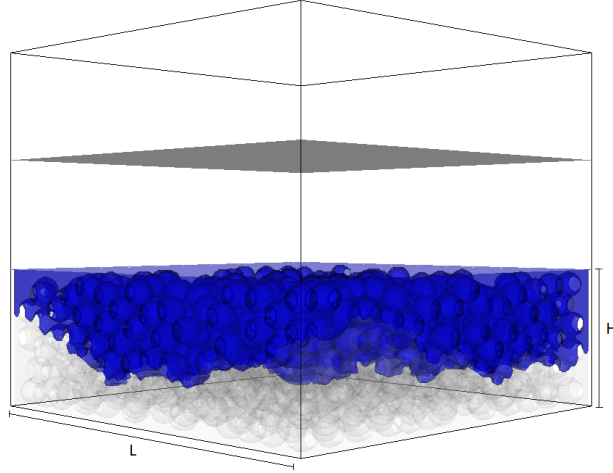


Figure 2: Domain for $\phi = 5.1$ with infiltration.

2.2.2. Boundary conditions

The boundary conditions used in all simulations in this work consist of the following: the upper and lower boundaries are periodic, the transverse boundaries are symmetric. The driving force for the flow is applied in the vertical direction. The porous medium is bordered by walls however the rest of the domain as the transverse boundaries is open.

2.2.3. Grid convergence study

To facilitate the evaluation of appropriate spatial resolution 4 grids are generated for $\phi = 6.7$ with a varying number of lattice nodes in the vertical (NH) and horizontal (NL) directions, the details of which are presented in

Table 2. A grid resolution test is undertaken using the generated grids. This

Table 2: Lattice node quantities for several grid resolutions.

	NH	NL	Total Nodes	$\Delta Cell[mm]$	d [lattice nodes]
Grid 1	50	150	1.125×10^6	0.1000	7.4
Grid 2	60	180	1.994×10^6	0.0833	8.9
Grid 3	70	210	3.087×10^6	0.0714	10.4
Grid 4	80	240	4.608×10^6	0.0625	11.8

276

277 test is run using single-phase isothermal air flow driven by gravity. The
 278 determination of grid resolution accuracy is accomplished by evaluating the
 279 relative error of the dimensionless permeability

$$K^* = K/d^2 = \frac{\bar{U}_z \mu_g}{(\rho_g g) d^2}, \quad (15)$$

280 where K is the permeability, \bar{U}_z is the mean vertical velocity, μ_g is the gas
 281 dynamic viscosity, ρ_g is the gas density, and g is gravitational acceleration.
 282 The permeability is evaluated only on the inner 2/3 of the geometry in the
 283 lateral direction to eliminate the contribution of the side wall effect as noted
 284 by Galindo-Torres et al. [32]. It should be here noted that all the quantities
 285 computed in this study are referred to this reduced volume in order to ensure
 286 that the side walls does not affect the results. The two-phase flow dynamics
 287 in porous media is determined by the balance of gravitational and capillary
 288 forces. Therefore, the dimensionless permeability in the grid resolution test
 289 is computed at a fixed characteristic gas capillary number $Ca_g = \rho_g g d^2 / \gamma$,
 290 where γ is the surface tension used in the multiphase simulations. Table 3
 291 presents the analysis of the grid resolution study and Grid 3 is chosen for all
 292 subsequent simulations as an acceptable compromise between the relative dif-

293 ference of refinement and computational requirement. The relative difference
 294 of dimensionless permeability is calculated over successive grid refinements
 295 as:

$$\% \text{ Difference} = \frac{\text{Permeability}_{\text{Grid } i+1} - \text{Permeability}_{\text{Grid } i}}{\text{Permeability}_{\text{Grid } i}}. \quad (16)$$

Table 3: Grid resolution test case input and results.

Case	g [lattice units]	Re [-]	Permeability [-]	% Difference
Grid 1	6.53E-5	0.00514	0.00539	-
Grid 2	4.53E-5	0.00575	0.00500	7
Grid 3	3.30E-5	0.00634	0.00474	5
Grid 4	2.55E-5	0.00703	0.00466	2

296

297 The pore size analysis for the domains considered in this work shows the
 298 mean pore sizes range 0.25-0.35 mm which corresponds to approximately 4-6
 299 lattice units with the resolution defined by Grid 3 (see Figure 4). This is con-
 300 sidered a reasonable value for resolving pore scale transport, as for instance
 301 discussed by Succi [19]. Such an observation corroborates the findings of the
 302 present grid analysis and the choice of the resolution addressed as Grid 3 for
 303 our multiphase simulations.

304 2.2.4. Multiphase input data

305 Standing water is initialized within the domain directly above the porous
 306 medium. The standing water height h is used as a characteristic length due
 307 to its contribution as the body force by way of hydrostatic pressure.

308 Using the particle diameter and standing water height as well as the choice
 309 of lattice resolution we can convert all relevant quantities. The results are

310 categorized by two primary non-dimensional parameters; ϕ which is defined
 311 previously, and the Bond number

$$\text{Bo} = \frac{(\Delta\rho g)h^2}{\gamma}, \quad (17)$$

312 where g is the variable representing the gravitational component of the body
 313 force, $\Delta\rho = \rho_l - \rho_g$ is the phase density difference, and γ is the interfacial
 314 surface tension.

315 The Bond number represents the ratio of gravitational and surface tension
 316 forces. Work by Slobozhanin et al. showed that for Bond numbers from 0 to
 317 5 there is little difference in the capillary pressure in tightly packed spheres
 318 [34]. Moreover if the Bond number is below 0.1 the effect of gravity can be
 319 neglected entirely.

320 A statistical analysis of meteorological data taken from Gothenburg, Swe-
 321 den and provided by Swedish Meteorological and Hydrological Institute (SMHI)
 322 is used to determine the standing water height and consequently the Bond
 323 numbers used in this study. The statistical analysis of hourly weather data
 324 taken over the period 1995.08.04 - 2018.05.01 is used to determine the aver-
 325 age rainfall intensity with the result being 2.5 mm/hr when rainless periods
 326 are discarded. This value is taken as the equivalent standing water height
 327 when the Bond number is 1. Since we are interested in rainfall events caus-
 328 ing flooding this number is increased two and threefold for our simulations,
 329 analogous to a scenario where extreme rainfall occurs over a short period of
 330 time and surface water is present. This corresponds to Bond numbers of 3.96
 331 for a standing water height of $h = 5.0$ mm and 8.92 when $h = 7.5$ mm.

332 In Table 4 the physical and lattice unit values for all input parameters
333 required for the simulations are listed. Table 5 identifies the 6 cases of the
334 study in terms of ϕ and Bo.

335 An additional parameter is required for implementing the multiphase sim-
336 ulations; the contact angle. Measurements by Ramírez-Flores et al. [35],
337 Schrader and Yariv [36], and Fér et al. [37] demonstrate the variability of
338 the contact angles with regard to soil aggregates and clay minerals. We moti-
339 vate our choice of 82° by noting that this value lies within the range of values
340 reported in experimental work. As reported in Fér et al. clay-coated mate-
341 rials exhibit a contact angle around 80° and the value decreases over time.
342 While a singular equilibrium value is set, a dynamic contact angle arises from
343 the simulation due to the presence of external forcing from gravity. A more
344 complicated modeling of the contact angle is neglected on the grounds that
345 we do not expect significant variations in the contact angle due to the low
346 flow velocity of the system [38].

Table 4: Physical and non-dimensional input parameters. The physical time is computed via the equivalence between physical and lattice units, i.e. $t = t_{LB} (L^2/L_{LB}^2) (\nu_{LB}/\nu_l)$.

Parameter	Variable	Value	Physical value	Physical unit
Porous medium height	H	70	5.0	[mm]
Standing water height	h	70, 105	5.0, 7.5	[mm]
Particle diameter	d	10.4, 6.9, 13.8	0.74, 0.494, 0.986	[mm]
Horizontal domain length	L	210	15	[mm]
Liquid dynamic viscosity	μ_l	2.4/6	1.00e-3	[Ns/m ²]
Gas dynamic viscosity	μ_g	0.12/6	1.68e-7	[Ns/m ²]
Liquid kinematic viscosity	ν_l	1/6	1.00e-6	[m ² /s]
Gas kinematic viscosity	ν_g	1/6	1.27e-5	[m ² /s]
Liquid density	ρ_l	2.4	998	[kg/m ³]
Gas density	ρ_g	0.12	1.20	[kg/m ³]
Surface tension	γ	0.093	0.073	[N/m]
Gravity	g	3.3e-5	9.8	[m/s ²]
Time	t	1	8.5×10^{-4}	[s]

Table 5: Case specifications.

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6
ϕ	6.7	10.1	5.1	6.7	10.1	5.1
Bo	8.92	8.92	8.92	3.96	3.96	3.96

3. Results and discussion

In Figure 3, saturation Sat is plotted as a function of dimensionless time for $Bo = 8.92, 3.96$. The dimensionless time is defined as

$$t^* = \frac{t}{\sqrt{\frac{h}{g}}}. \quad (18)$$

The saturation Sat is calculated by summing the liquid nodes in the porous medium and dividing by the total void node quantity. In the Shan-Chen method, the liquid-gas spatial transition is represented with a smooth diffusive interface. A computational node belongs to the liquid node when its

density overcome a specific threshold. This threshold is taken in our simulations as $\sqrt{2}$, a value that corresponds to the metastable state of the non-ideal equation of state.

In Figure 3 the infiltration for all values of ϕ displays a trend with a slope ≤ 0.5 in logarithmic scale. The slope 0.5 corresponds to the theoretical solution of Washburn's equation [39] which describes the relationship between penetration length l_p of a liquid into a fixed-radius capillary tube over time without gravitational forces. The equation relates the penetration length to a diffusive coefficient D_c and time as

$$l_p = (D_c t)^{\frac{1}{2}}. \quad (19)$$

Washburn's equation does not take into account gravity and describe the capillary rise of the liquid driven by the hydrophilicity of the material; the diffusive coefficient is a function of the pore radius and the hydrophilic contact angle. Instead, in our case, the hydrophilicity of the material can be neglected, because the contact angle is close to 90° , and gravity is the force that drives liquid penetration. In this conditions, when a liquid volume penetrates a single tubular pore under pressure or gravitational forcing, an analogous formulation to Eq. (19) can be derived, with the diffusive coefficient depending on the pore radius and the gravitational force.

When we consider the liquid penetration into a porous complex structure, the physical description is more complicated, given the intricate pore network that the liquid is forced to follow during imbibition. In some pores, slow liquid infiltration induced by the intricate topology of pores boundaries can

376 be observed. The infiltration can also be intermittent, as recently observed in
 377 experiment of two-phase flows into rock samples [40], especially at low values
 378 of porosity and Bond numbers, as the ones considered in this study. In such
 379 cases, liquid infiltration in some pores can be mathematically described by
 380 a power law similar to (19), but with a smaller exponent. Therefore, at the
 381 macroscopic scale, on average, the saturation of the porous medium follows
 382 a law as:

$$Sat(t) \propto (D_c t)^{\alpha(t)}. \quad (20)$$

383 In this formulation the diffusive coefficient is determined by the hydraulic
 384 pressure and the porous microstructure and alpha is a time-dependent expo-
 385 nent $\alpha(t) \leq 0.5$. The saturation curves in Figure 3 follow this mathematical
 386 description.

387 All the curves present a slow infiltration at short and long times while at
 388 intermediate times, they exhibit the highest infiltration rate. The differences
 389 in initial saturation are due to the particle packing at the surface which
 390 is not uniform for all cases. We see clearly in the mid-range saturation
 391 values that $\phi = 10.1$ behaves similarly to Eq. (20) with slope 0.5 indicating
 392 a flow behavior similar to a single pore penetration. When $\phi = 6.7$ the
 393 infiltration is less efficient in terms of saturation and it further decreases
 394 for $\phi = 5.1$. Furthermore, as seen in Figure 3, the decreased hydraulic
 395 pressure has an adverse effect on the infiltration. It is important to note
 396 that when saturation approaches 0.7 – 0.9 the values almost stagnate for
 397 several of the cases. This indicates some form of infiltration reduction within

398 the porous medium that is not heavily dependent upon the flow itself but
 399 rather the porous microstructure. We will discuss in the next subsection
 400 this result by categorizing the different geometries by their microstructure.
 401 Interestingly, it can be also noted that the infiltration rate appears to decrease
 402 with time, as the liquid approaches the bottom of the medium, where the
 403 spatial distribution of solid particles is significantly affected by the bottom
 404 layer where they lean. This observation is indeed further confirmed by noting
 405 that the infiltration rate between the different cases is lower for low values
 406 of ϕ , therefore when the packing effects are more pronounced.

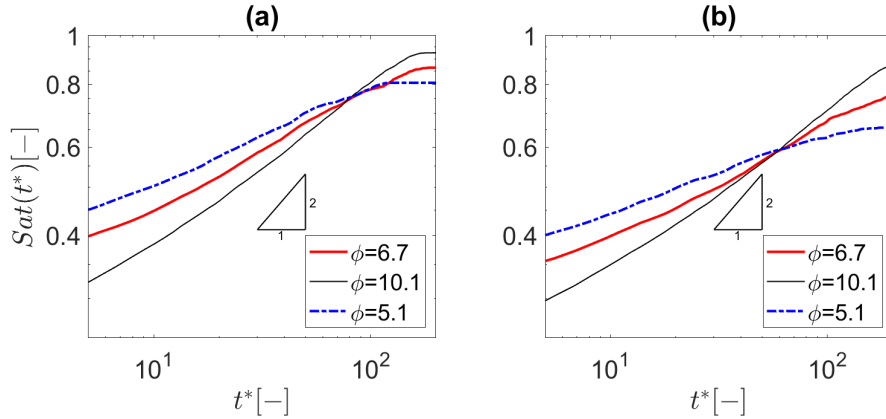


Figure 3: (a) Log-linear plot of saturation as a function of dimensionless time for $\phi = 6.7, 10.1, 5.1$ with $Bo = 8.92$. (b) Log-linear plot of saturation as a function of dimensionless time for $\phi = 6.7, 10.1, 5.1$ with $Bo = 3.96$.

407 3.1. Porosity as a function of porous medium depth

408 In Figure 4 the planar porosity orthogonal to the primary flow direction
 409 is plotted as a function of distance from the porous medium base ($H = 70$),
 410 measured in particle diameters d . At the base of the porous medium the
 411 particles are more ordered and we can see the uniformity in the packing over
 412 the first 3 particle diameters. This oscillatory effect is lost thereafter until the

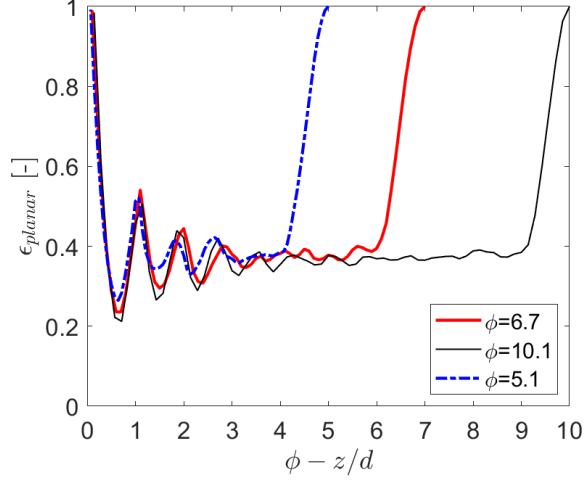


Figure 4: Flow-normal planar porosity ϵ_{planar} as a function of particle diameters d from porous medium base for $\phi = 6.7, 10.1, 5.1$.

413 surface is reached and the porosity decreases rapidly. It is clear from Figure
 414 4 the change in porosity is heavily correlated to the position relative to the
 415 particle packing itself. We also observe that the maximum saturation values
 416 showed in Figure 3 are connected with the change in porosity. In fact, these
 417 values are $\max(Sat) \approx 0.8, 0.85, 0.9$ for $\phi = 5.1, 6.7, 10.1$ which implies that
 418 the infiltration rate is dramatically reduced when the liquid front approaches
 419 the bottom at a distance of approximately one particle diameter; this occurs
 420 right before the last particle layer. By looking at Figure 4 we notice that
 421 in the interval over the last particle layer the value of porosity exhibits a
 422 sudden increase. This observation suggests that pore throat expansions can
 423 act to impair liquid infiltration. In Subsection 3.3 we will confirm that this
 424 anomalous behaviour is induced by the rapid change of the morphology of the
 425 microstructure. More detailed quantification of the porous microstructure as
 426 a function of position in the medium requires a characterization of individual

427 pores themselves.

428 3.2. Pore size distribution and infiltration depth

429 In order to better characterize the porosity, individual pore size distri-
430 butions have been calculated and the mean and standard errors at each
431 depth within the medium calculated. Note that while the geometries are 3-
432 dimensional it is difficult to accurately determine and characterize pore sizes
433 in 3 dimensions, though attempts have been made, such as by Suh et al. [15]
434 and Liu et al. [16]. We have opted for characterization by analyzing pore
435 sizes in the plane lying perpendicular to the primary flow direction. This is
436 accomplished by taking slices of the domain at specific depths and utilizing
437 image analysis to extract equivalent diameters of the pores. The equivalent
438 diameter command returns the diameter d_{pore} of a circle with the equivalent
439 area as the imaged pore A_{pore} , using the equation

$$d_{pore} = \sqrt{\frac{4A_{pore}}{\pi}}. \quad (21)$$

440 The mean pore diameter and standard error are plotted in Figure 5 as a
441 function of distance from the porous medium base, measured in particle
442 diameters, exactly as in Figure 4. The standard error is computed as

$$s_{\bar{x}} = \frac{s}{\sqrt{n}}, \quad (22)$$

443 where s is the sample standard deviation and n is the sample size.

444 There is a noticeable jump in the mean pore size for $\phi = 10.1$ at a single
445 particle depth from the bottom of the domain due to the packing. The jump

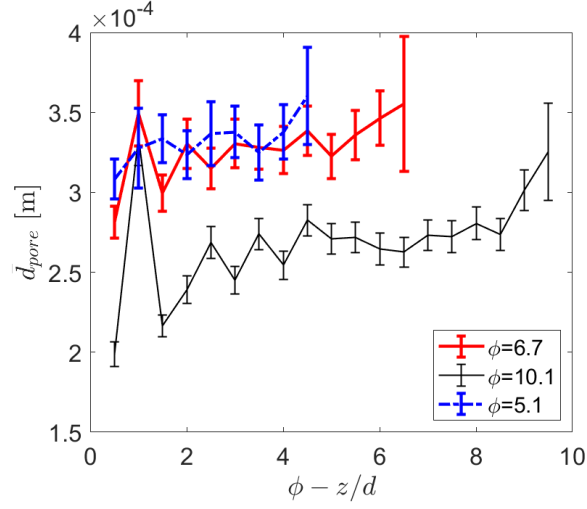


Figure 5: Pore diameter d_{pore} mean with standard error as a function of particle diameters d from porous medium base for $\phi = 6.7, 10.1, 5.1$.

446 is slightly less pronounced for $\phi = 6.7$ however there is little to no jump
 447 when $\phi = 5.1$. It should be noted that the values taken from the base of the
 448 medium are not shown as the mean pore sizes tend to infinity as porosity
 449 becomes 1. This reaffirms the oscillation of planar porosity seen in Figure
 450 4. If one looks at the standard errors for each particle sized there is a trend
 451 from less variation in the smallest particle size to higher variation for the
 452 largest particle size, meaning the distribution of pore sizes is wider for the
 453 larger particles. The standard errors averaged over the depth of the medium
 454 are $\overline{s_x} = 0.2, 0.14, 0.26$ for $\phi = 6.7, 10.1, 5.1$ respectively. This confirms the
 455 findings from the planar porosity analysis that the larger particle size and
 456 the uniformity of packing near the surface is relevant at the individual pore
 457 level. While the total porosity changes are similar, though not identical, the
 458 individual pore size changes are not as uniform in terms of magnitude.

459 As a consequence of higher variability in pore size distribution we expect

460 to see a less homogeneous flow pattern for a low value of the packing pa-
 461 rameter ϕ , i.e. when the size of the medium depth is comparable with the
 462 particle size. In Figure 6 the normalized infiltration depths are plotted for
 463 the smallest particle size $\phi = 10.1$ in (a) and the largest particle size $\phi = 5.1$
 464 in (b) at the same dimensionless time $t^* = 275$. This time was chosen as
 465 it clearly illustrates the difference in infiltration homogeneity between the
 466 different particle sizes. The penetration depth is determined by determining
 the deepest liquid node at each value in the flow-perpendicular plane.

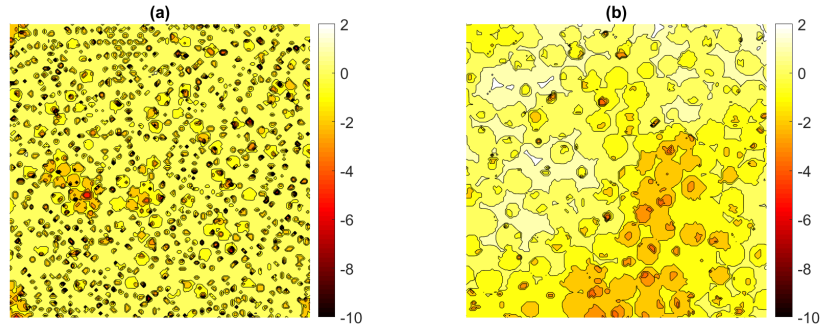


Figure 6: (a) Normalized distribution of liquid infiltration at $t^* = 275$ for $\phi = 10.1$. (b) Normalized distribution of liquid infiltration at $t^* = 275$ for $\phi = 5.1$. The color indicates standard deviations from the mean. $Bo = 3.96$.

467

468 By examining the normalized penetration depths for Figure 6 (a) and (b)
 469 we can see a marked difference in homogeneity of the flow. This agrees with
 470 the supposition that a wider variability of pore sizes in a thin medium can
 471 be linked directly to flow pathing preference, or ganglia formation. Ganglia
 472 here refers to finger-like structures comprised solely of liquid that penetrate
 473 farther into the microstructure than the bulk flow. In other words, it indicates
 474 an heterogeneous liquid front. Another quantification of the homogeneity of
 475 the water infiltration is given in Figure 7 where the probability distribution

functions (PDFs) for the infiltration depth are plotted. The timestep $t^* = 240$ is used when $Bo = 8.92$ due to the liquid reaching the base of the domain at higher time values for $\phi = 10.1$.

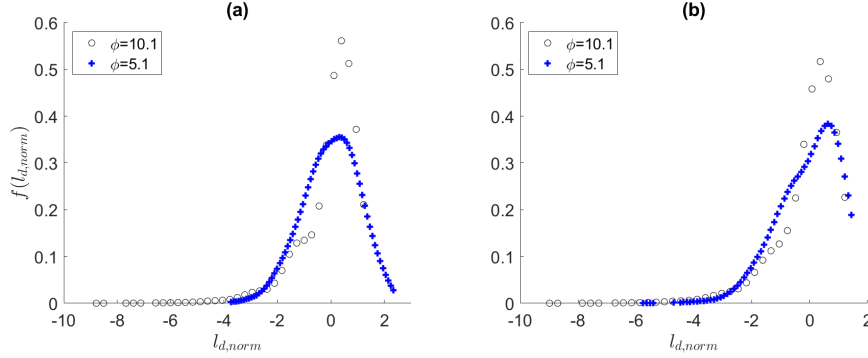


Figure 7: (a) PDF $f(l_{p,norm})$ of normalized liquid infiltration $l_{p,norm}$ at $t^* = 275$ for $\phi = 10.1, 5.1$ and $Bo = 3.96$. (b) PDF $f(l_{p,norm})$ of normalized liquid infiltration $l_{p,norm}$ at $t^* = 240$ for $\phi = 10.1, 5.1$ and $Bo = 8.92$. The x-axis indicates standard deviations from the mean.

The curves in both Figure 7 (a) and (b) indicate a larger distribution when $\phi = 5.1$ as seen from Figure 6 whereas the flow is highly homogeneous when $\phi = 10.1$ as seen by the high peaks at the mean value. A final point to be made is that the value of the Bond number does not radically change the infiltration pattern, thus enforcing the notion that the behaviour is not dependent primarily on the hydraulic head. With regard to the relationship between pore sizes and infiltration homogeneity it is highly likely the pore sizes themselves have a high impact on the infiltration dynamics. This is due to the energy required to fill the pores. This phenomena can be investigated by analyzing the liquid-gas interfacial area for each particle size.

3.3. Influence of liquid-gas interfacial area

Figure 8 gives the dimensionless liquid-gas interfacial area for each geometry as a function of dimensionless time. The clearest visible trends within the figures are the general slopes for all cases. When $\phi = 10.1$ and $\phi = 6.7$ we see a decrease over time in interfacial area for both hydraulic heads. The slope of the $\phi = 5.1$ case seems instead to oscillate around a constant value. The overall oscillation in interfacial area is indicative of liquid buildup at pore throat and subsequent sporadic jumping patterns of pore saturation. The $\phi = 5.1$ case displays small fluctuation amplitudes, suggesting slower infiltration in time.

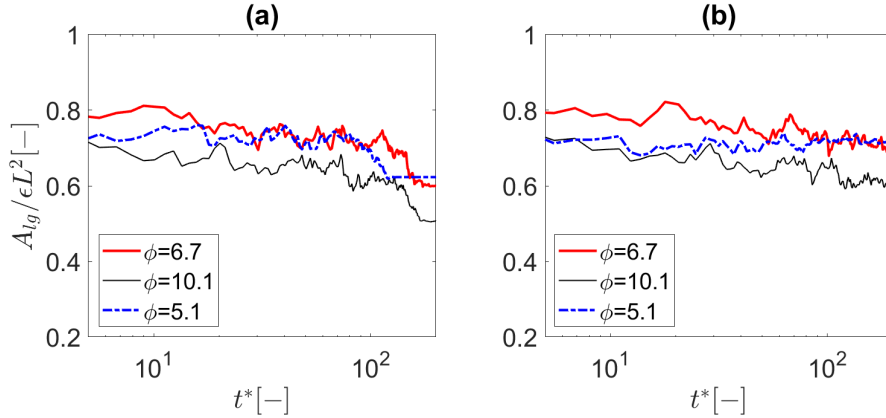


Figure 8: (a) Dimensionless liquid-gas interfacial area $A_{lg}/\epsilon L^2$ as a function of dimensionless time t^* for $\phi = 6.7, 10.1, 5.1$ with $Bo = 8.92$. (b) Dimensionless liquid-gas interfacial area $A_{lg}/\epsilon L^2$ as a function of dimensionless time t^* for $\phi = 6.7, 10.1, 5.1$ with $Bo = 3.96$.

The underlying cause of the intermittent behaviour of liquid-gas area buildup and possible stagnation lies in the balance of forces acting in the capillary structure and has been mathematically described firstly by Cassie and Baxter [18] for describing the mechanical balance responsible for the behaviour of droplets leaning on rough surfaces. The same concept has been

504 applied for describing the rapid pore-scale displacement known as Haines
 505 jump [41]. We can formalize such a force balance by applying the principle
 506 of Helmholtz free energy F which describes the thermodynamic balance of a
 507 isochoric and isothermal system as in (23).

$$dF = \delta W < 0 \quad (23)$$

$$= - \sum_{i=l,g} p_i dV_i + \gamma dA_{lg} \quad (24)$$

$$= -(p_l - p_g) dV_l + \gamma dA_{lg} \quad (25)$$

$$= -p_c d(Sat V_f) + \gamma dA_{lg} \quad (26)$$

$$dF^* = -\frac{p_c V_f}{\gamma} + \frac{dA_{lg}}{dSat} < 0 \quad (27)$$

$$V_f = \epsilon V_{tot} \quad (28)$$

508 where p_l, p_g, p_c are the liquid, gas and capillary pressure, respectively; V_l, V_f, V_{tot}
 509 are the liquid, total void, and total volume; and A_{lg} is the liquid-gas inter-
 510 facial area. Applying the concepts of thermodynamics of surface tension
 511 we rewrite Eq. (23) as Eq. (24). This equation represents the maximum
 512 amount of reversible work done by such a system, and with a few algebraic
 513 manipulations the resulting relation is given in Eq. (27).

514 This equation clearly shows the relationship between the interfacial area
 515 derivative and capillary pressure. This relationship determines the energy
 516 balance of the system: in presence of an interfacial area expansion, the cap-
 517 illary pressure term must compensate to facilitate liquid infiltration. This
 518 energy requirement can explain why drastic expansions, as the one induced
 519 by the packed microstructure at the bottom of the medium, can considerably

520 reduce infiltration rate and possibly impede it. The continuous liquid buildup
 521 at the pore throat and rapid pore invasion mechanisms induced by packed
 522 microstructures give rise to intermittent infiltration behaviour at pore-level
 523 and anomalous reduced infiltration rate at the macroscopic scale.

524 Thus to further evaluate this formalized requirement we plot in Figure 9
 525 the interfacial area as a function of saturation for all cases. In Figure 9(a)
 526 and 9(b) where infiltration occurs the general slope is negative so that the
 527 inequality in Eq. (27) is easily satisfied and infiltration occurs uniformly. In
 528 Figure 9(c) it is clear that especially under lower hydraulic pressure the area
 529 does not significantly decrease with saturation, indicating that Eq. (27) is
 530 possibly not satisfied in some pores and total infiltration of the medium is
 531 slowed down. In addition, infiltration fails when the area-saturation deriva-
 532 tive is not sufficiently steep after some small initial increase. When this
 533 derivative condition is reached infiltration occurs, however this condition
 534 must be maintained for increasing saturation for the process to continue. If
 535 the interfacial area increment is too large to be sustained by the capillary
 536 pressure, infiltration will stop causing the packed bed to act like a capillary
 537 barrier.

538 Ross (1990) discussed capillary barriers and determined criteria for their
 539 size and liquid deflection capacity in analytical terms [17] in context of their
 540 diversion capacity. Diversion capacity in this case refers to the amount of
 541 liquid that can be channeled in a lateral direction by the interaction be-
 542 tween an upper and lower layer of different sized particles. It is important to
 543 note that while the effect has been noted and studied, the conditions for the
 544 phenomenon to affect the infiltration process from a morphological perspec-

tive have not been quantified, to the best knowledge of the authors. This
 phenomenon clearly plays a role in infiltration dynamics, even when contact
 angles are near neutral. The morphological impact on liquid infiltration is
 expected to increase when the contact angle is reduced; thus quantifying its
 influence is of importance for cases with variable saturation, as is the case
 with rainfall infiltration of soils. Additional work must be undertaken to
 more accurately capture the pore size and distributions since the current
 method only characterizes them in a planar manner. A direct comparison of
 capillary pressure and the interfacial area-saturation derivative would be ap-
 propriate to validate the applicability of the equation and could be a critical
 aid in deriving conditions for infiltration failure.

3.4. *Design considerations*

From a design perspective we show the results of the six cases in this
 study in terms of the infiltration rate in Figure 10 and offer some insight
 into how these results can be applied in practice. This rate is quantified
 by α which is the exponent of the power law given in (20), at intermediate
 times. α can be considered as a measure of the ability of the microstructure
 to detain the infiltrating rainfall, with higher values corresponding to more
 rapid infiltration and shorter detention time. Therefore it is recommended
 to consider the microstructure with regard to depth and particle size in the
 design of a green roof, particularly when including thin substrate layers,
 when the thickness of the medium and the particle size are of the same
 magnitude. As we have seen in this study, larger particle sizes in relation to
 the porous media thickness may reduce infiltration as opposed to a substrate

569 consisting of smaller particles; this phenomenon being exacerbated by lower
570 rainfall intensities. In addition there is merit in considering the climatic
571 conditions in the location of installation as by taking local rainfall quantities
572 into account in the design, it is possible to optimize the roof performance
573 for extreme conditions where the benefit of a green roof is maximized. It is
574 also possible to layer different particle thicknesses so as to create a substrate
575 that is designed to perform optimally under variable conditions. By layering
576 substrates in this way one can achieve the desired detention of rainfall in the
577 green roof. This may be the most important takeaway from this study in
578 regards to designing green roofs for variable climatic conditions in the most
579 efficient way.

580 If one considers how these results can be combined with previous research
581 into green roof performance there are a few points to consider. Firstly, we
582 stress here that we have considered only the growth substrate and no veg-
583 etation is included. Blue roofs do not include vegetation and are primarily
584 used for storm water management thus our results are directly applicable to
585 such constructions. If vegetation is included we must consider the mechan-
586 ical blocking effect at the surface however this simply reduces the quantity
587 of surface water for infiltration. In addition, root networks will disturb the
588 soil matrix and contribute to small channels throughout the medium where
589 liquid can flow more easily. These channels may contribute to areas in the
590 substrate where liquid will not reach as frequently and will be more hy-
591 drophobic. From a larger time scale the impact of evapotranspiration must
592 be considered, however this process primarily affects the detention capacity
593 of a green roof as it removes trapped water from the smallest pores rather

594 than the liquid able to infiltrate and drain out of the soil. Most green roof
595 constructions also include a drainage layer directly beneath the root barrier
596 layer and growth substrate layer. This means that at the base of the growth
597 substrate the packing will resemble the physics where wall impacts will be
598 significant. By applying the results presented here one can design the lowest
599 particle layers in contact with the root barrier (wall) to facilitate the transfer
600 of water from the growth substrate to the drainage layer. By combining the
601 purely mechanical processes such as those studied in this work with the con-
602 tribution from evapotranspiration we can generate a more accurate picture
603 for designers that captures many factors critical to the performance of green
604 roofs over singular rainfall events and over the longer term.

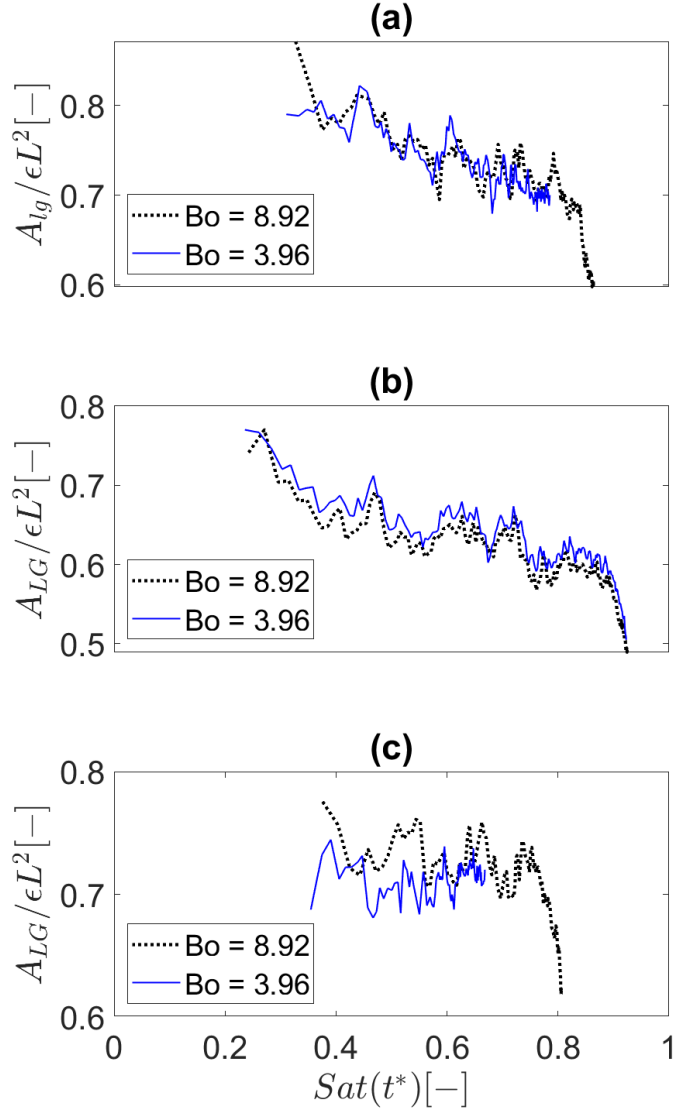


Figure 9: Dimensionless liquid-gas interfacial area $A_{lg}/\epsilon L^2$ as a function of saturation $Sat(t^*)$ for $\phi = 6.7$ (a), $\phi = 10.1$ (b), and $\phi = 5.1$ (c).

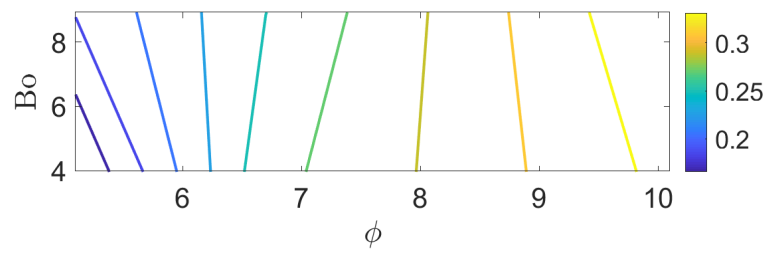


Figure 10: α extracted at intermediate times from Figure 3 plotted as a function of ϕ and Bo .

605 4. Conclusion

606 In this paper we have explored the effect of the microstructure on liquid
607 infiltration into thin unsaturated porous media. Three microstructures de-
608 fined by a unique packing parameter ϕ have been evaluated and infiltration
609 is driven by 2 Bond numbers, representing different standing water heights
610 on the porous medium surface. We have demonstrated the relationship be-
611 tween the microstructure and the flow homogeneity by analyzing saturation,
612 liquid-gas interfacial area, pore size distribution, porosity, and infiltration
613 depth. It is shown that the liquid-gas interfacial area plays a significant
614 role in infiltration and is determined by the microstructure thickness in re-
615 lation to the particle sizes. The analysis showed that while the total planar
616 porosity of each domain remained similar, the effect of particle size in the
617 homogeneity of the layering impacted the infiltration. This is due to the
618 larger variation of pore sizes found in the domains with larger particles sizes,
619 leading to increased inhomogeneous flow patterns. This result is formalized
620 by applying the concept of Helmholtz free energy to liquid infiltration of a
621 porous medium as the energy balance between capillary pressure and liquid-
622 gas interfacial area. This balance is instrumental in determining the flow
623 pattern within the microstructure as is dependent upon the structure itself.
624 This behavior can be controlled by layering different microstructures within
625 green roof substrates to optimize their performance with regard to rainfall
626 detention time.

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